

Anomalous Energy Transport across Topological Insulator Superconductor Junctions

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We study the nonequilibrium energy transport across a topological insulator/superconductor junction, by deriving an interfacial heat current formula through scattering wave approach. Several anomalous thermal properties are uncovered, such as thermal energy's Klein tunneling, asymmetric Kapitza resistance and negative differential thermal resistance. We expect these findings could have potential applications for the energy control in various hybridized mesoscopic systems.

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Topological insulators (TIs), characterized by a bulk gap and a gapless surface mode with a Dirac-like linear dispersion, are presently one of the most interesting topics in condensed matter physics [1, 2]. Their conducting surface states in the insulating gap are topologically protected by time-reversal symmetry, hence robust to disorders and perturbations, potentially leading to various device applications. With the help of doping-induced superconductivity in TIs [3] or by depositing superconducting materials on TIs due to the proximity effect [4–6], the interplay between the superconducting ordering and the gapless chiral surface state has triggered much interest [2].

On the one hand, such topological insulator superconductor (TI/S) junctions have been used to create chiral Majorana fermions for topological quantum computations and for the study of their impacts on electronic tunneling properties [7–12]. On the other hand, in view of the fact that understanding thermal properties of hybrid mesoscopic structures is crucial for future quantum/nano technology [13], hybrid topological superconductor junctions could be a natural candidate for managing heat dissipation/refrigeration and controlling energy transport. It has the potential to open up a rich variety of thermal device concepts in superconducting-circuit-based systems, just like thermal diodes, thermal transistors, thermal logic gates and thermal memories in phononics [14].

In this Letter, we study the nonequilibrium energy transport across a TI/S junction interface and uncover its anomalous thermal properties, such as thermal energy's Klein tunneling, asymmetric Kapitza resistance and negative differential thermal conductance (NDTC). Among them, Kapitza resistance measures the interfacial thermal resistance when thermal energy flows through the interface between two different materials [15, 16]. Asymmetric Kapitza resistance is one unusual thermal property that the interface acts as a good thermal conductor if a positive thermal bias is applied, while with a negative thermal bias it exhibits poor thermal conduction, thus effectively acting as a thermal insulator. As such, it functions as a thermal rectifier or diode (for a review, see [14, 17]). While the NDTC, another unusual thermal transport phenomenon, where the heat current across a thermal conductor decreases when the temperature bias increases (for a review, see [14]), is an essential element for the construction of thermal transistors

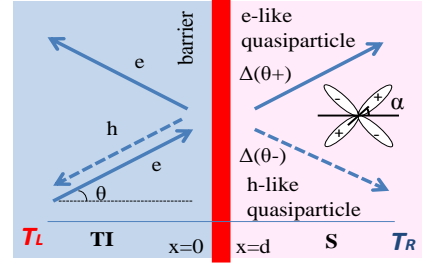


FIG. 1. (color online). Schematic illustration of the reflections and transmissions at the TI/S interfaces.

and thermal logic gates, and has been shown to exist in many nonlinear systems. We believe similar findings in superconducting hybridized mesoscopic junctions could extend the conceptual thermal devices in Phononics into superconducting-circuit based systems and have great potential applications [18] in the near future.

As depicted in Fig. 1, we consider a two dimensional (2D) TI/S junction attached to their respective thermal reservoirs at T_L and T_R , with an insulating barrier locating at $x \in [0, d]$. The 2D TI junction part ($x < 0$) could be formed on the surface of 3D topological insulators, the S junction part ($x > d$) could be induced via the proximity effect, and the barrier (B) part could be constructed by gating voltage or doping. We assume the same Fermi level in both TI and S, and employ the Bogoliubov-de Gennes (BdG) equation $\hat{H}\psi = E\psi$ to study the thermal transport properties. The Hamiltonian of the surface state on the topological superconductor is given by

$$\hat{H} = \begin{pmatrix} \hat{H}_0(\mathbf{k}) - E_F & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{H}_0^*(-\mathbf{k}) + E_F \end{pmatrix} \quad (1)$$

acting on a Nambu basis $(\psi_{e\uparrow}, \psi_{e\downarrow}, \psi_{h\uparrow}, \psi_{h\downarrow})$, with $\hat{H}_0(\mathbf{k}) = \hbar v_F(k_x \hat{\sigma}_y - k_y \hat{\sigma}_x) + U_0 \Theta(x) \Theta(d - x)$ and $\hat{\Delta} = i \hat{\sigma}_y \Delta(\theta, T) \Theta(x - d)$. Here, v_F is the Fermi velocity, $\hat{\sigma}_{x(y)}$ denote Pauli matrices, U_0 is the barrier potential and $\Delta(\theta, T)$ depicts the order parameter with a given pairing symmetry and temperature dependencies. Throughout the work, we consider $E_F \gg (|\Delta|, E)$ to satisfy the mean-field nature of BdG approach, *i.e.*, the superconducting coherence length $\hbar v_F / |\Delta|$

is much larger compared to the Fermi wavelength $\hbar v_F/E_F$. Adjusting E_F can be achieved via doping or gate voltage.

Since in superconductor junctions, the quasiparticles are carriers of thermal energy, we need to obtain the transmission (equivalently the reflection) coefficients of quasiparticles in order to investigate the thermal transport properties. Considering the conservation law for particle current, we can simplify the problem by merely considering the particle (including both electron and hole) current in the side of TI. Defining $f = \begin{pmatrix} \psi_{e\uparrow} \\ \psi_{e\downarrow} \end{pmatrix}$ and its hole counterpart $g = \begin{pmatrix} \psi_{h\uparrow} \\ \psi_{h\downarrow} \end{pmatrix}$, we have the probability density for finding either an electron or a hole, $P = |f|^2 + |g|^2$. By using the BdG equation $i\hbar\partial_t \begin{pmatrix} f \\ g \end{pmatrix} = \hat{H} \begin{pmatrix} f \\ g \end{pmatrix}$ with Eq. (1), and considering the continuity equation $\partial_t P + \nabla \cdot J_P = 0$, we obtain the x -component of the particle current:

$$J_P^x = v_F(f^\dagger \hat{\sigma}_y f - g^\dagger \hat{\sigma}_y g). \quad (2)$$

Note the hole current is a time-reversed counterpart of the electron contribution so that it naturally obtains an opposite sign compared with the electron current. If we express the whole wave function at the TI side in terms of the normal reflection amplitude, b , and Andreev reflection [19] (for electron-hole conversion) amplitude a , which will be defined explicitly below, the particle current can be written as

$$J_P^x(E, \theta) = 2v_F \cos \theta (1 - |a(E, \theta)|^2 - |b(E, \theta)|^2). \quad (3)$$

This expression of the particle current has a clear physics picture that $\tilde{\kappa}(E, \theta) := 1 - |a(E, \theta)|^2 - |b(E, \theta)|^2$ denotes the transmission of energy carriers with energy E and incident angle θ , $v_F \cos \theta$ the effective velocity in the x direction and 2 the spin degeneracy. Considering the carrier's energy E , the Fermi occupation difference between two sides of the interface $f_L - f_R = \frac{1}{e^{E/k_B T_L} + 1} - \frac{1}{e^{E/k_B T_R} + 1}$ and summation over all possible incidence angles and momenta $\sum_{k_x} \int_{-\pi/2}^{\pi/2} d\theta = \int dE \int_{-\pi/2}^{\pi/2} d\theta (dE/dk_x)^{-1} = \int dE \int_{-\pi/2}^{\pi/2} d\theta \frac{1}{\hbar v_F \cos \theta}$, we arrive at the energy current expression:

$$J_Q = \frac{2}{h} \int_{-\infty}^{\infty} dE E \kappa(E) [f_L - f_R], \quad (4)$$

with $\kappa(E) = \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \tilde{\kappa}(E, \theta) = \int_{-\pi/2}^{\pi/2} d\theta \cos \theta (1 - |a|^2 - |b|^2)$. Note that this expression is general and is obtained before solving the reflection coefficients a, b . In fact, similar expressions of the energy current in topological-trivial metal superconductor junctions have been obtained by the rigorous derivation through linear response of entropy production [20] or by heuristic argument [21]. It is worth emphasizing that all the transports considered in this work are charge neutral, *i.e.*, the carriers transport only thermal energy without charge current. In fact, if we follow the same procedure for charge transport, we will arrive at a similar expression for electric current: $J_e = \frac{2e}{h} \int dE \int d\theta \cos \theta \tilde{\sigma}(E, \theta) [f_L - f_R]$, with $\tilde{\sigma} = 1 + |a|^2 - |b|^2$, similar to the BTK formula [19, 22]. One can then get that since the even symmetry of $\tilde{\sigma}$ ($\tilde{\sigma}(E, \theta) =$

$\tilde{\sigma}(-E, \theta)$) and the odd symmetry of $f_L - f_R$ with respect to E , J_e vanishes as zero.

We now proceed to determine the scattering coefficients of Andreev reflection amplitude a and normal reflection amplitude b by imposing the boundary conditions on the wave functions at the interfaces of barrier. Diagonalizing Eq. (1) straightforwardly yields the wave functions in the TI, barrier, S regions. In the TI region ($x < 0$), for electrons and holes traveling the $\pm x$ direction with a conserved transverse momentum k_y and energy E measured from E_F , the wave functions are given as

$$\begin{aligned} \psi_{\text{TI}}^{e\pm} &= (1, \pm i e^{\pm i\theta}, 0, 0) e^{i(\pm k_x x + k_y y)}, \\ \psi_{\text{TI}}^{h\pm} &= (0, 0, i, \pm e^{\pm i\theta}) e^{i(\mp k_x x + k_y y)}, \end{aligned}$$

where $k_x = E_F \cos \theta / (\hbar v_F)$ and $\theta = \arcsin(\hbar v_F k_y / E_F)$ is the angle of incidence. Note we have used the condition $E_F \gg E$. In the barrier region ($0 < x < d$), we employ the thin barrier limit [23]: $d \rightarrow 0$, $U_0 \rightarrow \infty$ but with a constant product $Z \equiv U_0 d / (\hbar v_F)$, characterizing the strength of the insulating barrier, we then obtain

$$\begin{aligned} \psi_{\text{B}}^{e\pm} &= (1, \pm i, 0, 0) e^{i(\pm Zx/d + k_y y)}, \\ \psi_{\text{B}}^{h\pm} &= (0, 0, i, \pm 1) e^{i(\mp Zx/d + k_y y)}. \end{aligned}$$

In the S region ($x > d$), the electron-(hole-)like quasiparticles are mixtures of electrons and holes. Thus, the transmitted wave functions have the forms:

$$\begin{aligned} \psi_{\text{S}}^{e+} &= (1, i e^{i\theta}, -i \Gamma_+ e^{i(\theta - \phi_+)}, \Gamma_+ e^{-i\phi_+}) e^{i(k_x x + k_y y)}, \\ \psi_{\text{S}}^{h+} &= (\Gamma_-, -i \Gamma_- e^{-i\theta}, i e^{-i(\theta + \phi_-)}, e^{-i\phi_-}) e^{i(-k_x x + k_y y)}, \end{aligned}$$

where $e^{i\phi_{\pm}} = \Delta(\theta_{\pm}, T) / |\Delta(\theta_{\pm}, T)|$ with $\theta_+ = \theta, \theta_- = \pi - \theta$ and $\Gamma_{\pm} = v_{\pm} / u_{\pm}$, with $u_{\pm}^2 = \frac{1}{2}(1 + \sqrt{E^2 - |\Delta(\theta_{\pm}, T)|^2 / |E|}) = 1 - v_{\pm}^2$. For a d -wave pairing symmetry, $\Delta(\theta, T) = \Delta(T) \cos(2\theta - 2\alpha)$ with $\Delta(T) = \Delta_0 \tanh[(\pi k_B T_c / \Delta_0) \sqrt{0.953(T_c/T - 1)}]$ [24]. Here T_c is the critical temperature, Δ_0 denotes the superconducting gap at zero temperature and α is the angle between the normal direction of the barrier interface and the x axis of the $d_{x^2-y^2}$ -wave superconductor. By taking into account the boundary conditions:

$$\Psi_{\text{TI}}|_{x=0} = \Psi_{\text{B}}|_{x=0}, \quad \Psi_{\text{B}}|_{x=d} = \Psi_{\text{S}}|_{x=d},$$

with $\Psi_{\text{TI}} = \psi_{\text{TI}}^{e+} + b \psi_{\text{TI}}^{e-} + a \psi_{\text{TI}}^{h-}$, $\Psi_{\text{S}} = t_e \psi_{\text{S}}^{e+} + t_h \psi_{\text{S}}^{h+}$, $\Psi_{\text{B}} = r_1 \psi_{\text{B}}^{e+} + r_2 \psi_{\text{B}}^{e-} + r_3 \psi_{\text{B}}^{h+} + r_4 \psi_{\text{B}}^{h-}$, the Andreev and normal reflection coefficients are found to be

$$\begin{aligned} a &= \frac{-\cos^2 \theta \Gamma_+ e^{i(\theta - \phi_+)}}{\cos^2 \theta + \sin^2 \theta \sin^2 \theta (1 - \Gamma_+ \Gamma_- e^{i(\phi_- - \phi_+)})}, \\ b &= \frac{\sin Z \sin \theta (\cos Z \cos \theta - i \sin Z) (1 - \Gamma_+ \Gamma_- e^{i(\phi_- - \phi_+)})}{-e^{-i\theta} [\cos^2 \theta + \sin^2 \theta \sin^2 \theta (1 - \Gamma_+ \Gamma_- e^{i(\phi_- - \phi_+)})]}. \end{aligned}$$

Finally, using the obtained coefficients a and b , we get

$$\begin{aligned} \tilde{\kappa}(E, \theta) &:= 1 - |a(E, \theta)|^2 - |b(E, \theta)|^2 \\ &= \tilde{\kappa}_{\text{TI}} \frac{1 - \tilde{\kappa}_{\text{TI}} |\Gamma_+|^2 + (\tilde{\kappa}_{\text{TI}} - 1) |\Gamma_+ \Gamma_-|^2}{|1 + (\tilde{\kappa}_{\text{TI}} - 1) \Gamma_+ \Gamma_- e^{i(\phi_- - \phi_+)}|^2}, \quad (5) \end{aligned}$$

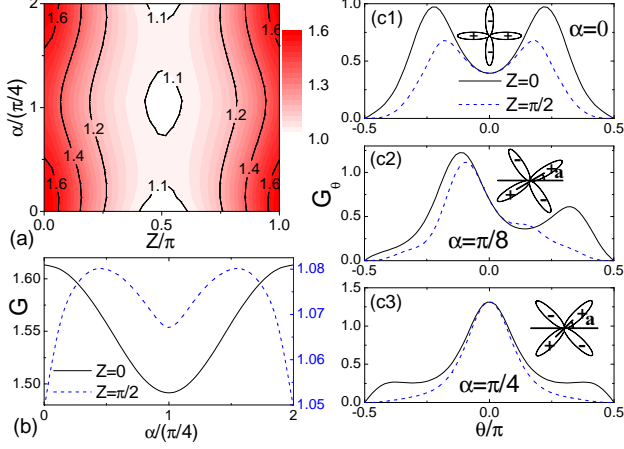


FIG. 2. (color online). Thermal energy's Klein tunneling. (a) Thermal conductance as a function of the barrier strength Z and the rotation angle α of the d -wave order parameter. (b) Intersections of (a) for $Z = 0$, and $\pi/2$. (c) Angle-resolved thermal conductance G_θ for different α and Z . Solid lines are for $Z = 0$ while dashed ones for $Z = \pi/2$. Parameters are $T = 70\text{K}$, $T_c = 116\text{K}$, $\Delta_0 = 30\text{meV}$. Thermal conductance G is in the unit of $\Delta_0 k_B/h$.

where

$$\tilde{\kappa}_{\text{TI}} := \tilde{\kappa}(|E| \gg \Delta_0, \theta) = \frac{\cos^2 \theta}{\cos^2 \theta + \sin^2 Z \sin^2 \theta} \quad (6)$$

is reminiscent of the relativistic Klein tunneling [25], as a consequence of the spin-orbit coupling in TIs. The barrier becomes transparent for the thermal energy transport at the resonance condition, $Z := \frac{U_0 d}{\hbar v_F} = n\pi$, $n = 0, \pm 1, \dots$ (such that $\sin Z = 0$), or at the normal incidence ($\theta = 0$).

In the linear response regime $T_L = T + \delta T/2$, $T_R = T - \delta T/2$, $\delta T \rightarrow 0$, we have the thermal conductance:

$$G := \frac{J_Q}{\delta T} = \frac{2}{h} \int_{-\infty}^{\infty} dE \int_{-\pi/2}^{\pi/2} d\theta \frac{E^2 \cos \theta \tilde{\kappa}(E, \theta)}{4k_B T^2 \cosh^2(\frac{E}{2k_B T})}. \quad (7)$$

As illustrated in Fig. 2(a), the oscillatory dependence of G on the barrier strength Z shows the Klein tunneling behavior of energy: thermal conductance anomalously increases when the barrier increases within $[(n+1/2)\pi, (n+1)\pi]$, consistent with the behavior of $\sin^2 Z$ in Eq. (6). G also has an oscillatory dependence on α , the rotation angle of the superconducting order parameter. As detailed in Fig. 2(b), when $Z = 0$, G monotonically decreases as α rotates from 0 to $\pi/4$, but when Z increases to $\pi/2$, G first increases and then decreases. This nonmonotonic behavior is due to the competition of Klein tunneling and superconducting order parameter (gap), which we explain below.

In the S part, thermal energy is carried by the quasiparticles, which only transport beyond the gap Δ , so that the smaller Δ , the larger thermal conductance. In other words, the rotation angle α adjusts G through adjusting the angle dependence of the superconducting gap. To further understand the competition between Klein tunneling and order parameter

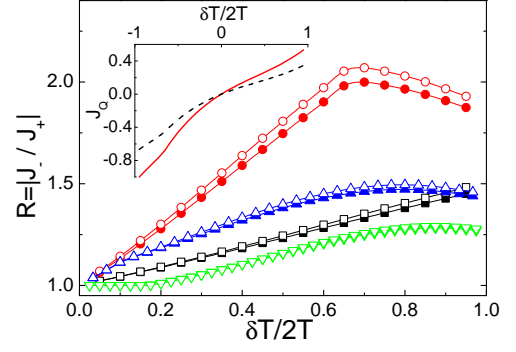


FIG. 3. (color online). Rectification ratios as a function of temperatures. Values apart from 1 indicate asymmetric Kapitza resistances. \blacksquare ($T = 35\text{K}$), \bullet ($T = 70\text{K}$), \blacktriangle ($T = 104\text{K}$), \blacktriangledown ($T = 140\text{K}$) denotes for $Z = 0$. Their hollow counterparts are for cases of $Z = \pi/2$. Inset shows one example of the J_Q profiles depending on temperature bias for $Z = 0$ (solid) and $\pi/2$ (dashed), at $T = 70\text{K}$. Other parameters are the same as in Fig. 2. The energy current J_Q is in the unit of Δ_0^2/h .

Δ , we define the angle-resolved thermal conductance G_θ as $G = \int_{-\pi/2}^{\pi/2} d\theta G_\theta$ and plot it as a function of the incidence angle θ in Figs. 2(c1-c3). For the case of $Z = 0$, when $\alpha = 0$, G_θ has two peaks around $\theta = \pm\pi/4$ where Δ is gapless; while, when α rotates to $\pi/4$, two peaks becomes a single peak around $\theta = 0$. As a result, G , the angle integration of G_θ , decreases as α increases from 0 to $\pi/4$. For α changing from $\pi/4$ to $\pi/2$, the behavior is symmetrically reversed. When the barrier Z increases, the Klein tunneling comes into play. For the case of $Z = \pi/2$, when $\alpha = 0$, although there are still two peaks for thermal conductance, their intensity is suppressed dramatically. When $\alpha = \pi/4$, the gapless angle coincides with the normal incidence angle, the barrier becomes transparent. Therefore, the Klein tunneling helps to keep the single conductance peak (at $\theta = 0$) intensity unchanged. At the intermediate regime $\alpha = \pi/8$, one peak near $\theta = 0$ preserves while the other peak far from $\theta = 0$ is repressed. As a consequence, the thermal conductance G increases first and then decreases within $\alpha \in [0, \pi/4]$.

The asymmetric Kapitza resistance is essentially a nonlinear response behavior. It is a consequence of different temperature responses of different materials at two sides of the interface [14]. The inset of Fig. 3 shows typical J_Q behaviors at $T = 70\text{K}$ for $Z = 0$ (solid line) and $\pi/2$ (dashed line), via varying temperature bias. As a measure of the asymmetry, we define the rectification ratio $R = |J_- / J_+|$, where J_+ refers to thermal current when $\delta T = T_L - T_R > 0$ while J_- refers to thermal current after switching the temperature bias $T_L \leftrightarrow T_R$. As shown in Fig. 3, when temperature bias is apart from 0, R becomes more deviating from 1. Except for the low temperature case, (e.g. $T = 35\text{K}$), other three examples show that increasing bias does not always increasing the rectification ratio at the large bias regime. The results also indicate that although the insulating barrier changes the J_Q profiles quite noticeably, it does not change the rectifica-

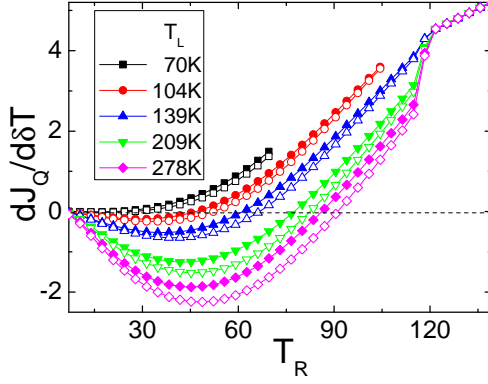


FIG. 4. (color online). NDTC for various temperatures at $Z = 0$ (filled symbols) and $Z = \pi/2$ (hollow symbols). Other parameters are the same as in Fig. 2. Results imply that the barrier can enhance the NDTC.

tion ratio significantly, which is even slightly enhanced by the barrier. In addition, R has a nonmonotonic temperature dependence that increasing T first increases and then decreases R , as exemplified by the highest curves for $T = 70\text{K}$ in Fig. 3. This is reasonable that the asymmetric Kapitza resistance in our system results from the different temperature responses of topological insulator and superconductor at the sides of the interface: At higher temperature, the superconducting gap diminishes so that the superconductor tends to topological insulator and both sides of the interface tend to have the same temperature response, which explains the reduction in R . At lower temperatures, although two sides of the interface have distinct temperature responses, the bias δT cannot be larger than T such that small bias reduces R . Therefore, the optimal R appears at intermediate temperature.

The superconductor is usually a bad thermal conductor since its gap Δ forbids the existence of quasiparticles that is responsible for the energy transport. Increasing the temperature T_R at the S part could increase the energy transmission $\kappa(E)$ (in Eq. (4)) by diminishing the superconducting gap to allow more thermal energy carriers, while simultaneously decrease the temperature bias $\delta T = T_L - T_R$ as well as the occupation difference $f_L - f_R = \frac{1}{e^{E/k_B T_L} + 1} - \frac{1}{e^{E/k_B T_R} + 1}$. Once the increased $\kappa(E)$ is able to compensate the loss in $f_L - f_R$ due to the decreased δT , we expect to observe NDTC, i.e., the energy current increases as the bias δT decreases. To characterize this anomalous behavior, we define the differential thermal conductance (DTC): $dJ_Q/d\delta T$, for given finite δT . Note that this is a nonlinear quantity similar to the nonlinear differential electrical conductance dI/dV , and is different from the previous defined thermal conductance G in Eq. (7), which is a linear quantity at $\delta T \rightarrow 0$. As a showcase, we calculate DTC in Fig. 4, with varying T_R in the S region but fixing T_L as a reference temperature. Indeed, NDTC appears as we expect, although it is absent for the low T_L case (e.g. $T_L = 70\text{K} > T_R$). Increasing T_L enhances the regime of NDTC. However, when T_R increases across a threshold and approaches to T_L , NDTC disappears. In addition, the insu-

lating barrier can also slightly enhance NDTC, as shown in Fig. 4. When the superconducting part is replaced with a topological insulator, there exists no NDTC.

In summary, using the scattering wave approach, we have derived an interfacial heat current formula in a TI/S junction. With the help of this formula, we have studied the nonequilibrium energy transport across this interfacial system and have uncovered several anomalous thermal properties for the TI/S interface, such as thermal energy's Klein tunneling, asymmetric Kapitza resistance and negative differential thermal resistance. We believe our results have revealed the potential applications of hybridized superconductor/topological insulator systems for the smart energy control at mesoscopic scales.

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